Equilibrium and Transport Properties of CO_2+NO and CO_2+N_2O Mixtures: a Molecular Simulation Study

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In the present study, the thermodynamic behaviour and transport properties of CO_2+N_2O and CO_2+NO mixtures have been investigated using molecular simulations. These simulations were based on Monte Carlo and Molecular Dynamics calculations using force fields calibrated on pure component properties, and no adjustment on mixture properties was performed. Original force fields have been developed for N_2O, NO and N_2O_2 molecules. Special care must be paid when studying systems containing nitric oxide because this compound can exist as a mixture of monomers (NO) and dimers (N_2O_2) under certain pressure and temperature conditions. Liquid-vapor coexistence properties of the reacting NO-N_2O_2 system were thus first investigated using combined reaction ensemble and Gibbs ensemble Monte Carlo methods. Using the new proposed force fields, phase compositions, phase densities and phase viscosities were then determined for CO_2+NOx mixtures. Due to the strong similarities between carbon dioxide and nitrous oxide (Tc (CO_2) = 304.21 K; Tc (N_2O) = 309.57 K; Pc (CO_2) = 7.38 MPa; Pc (N_2O) = 7.24 MPa), the obtained thermodynamic and transport properties for a CO_2+N_2O mixture with 10 mol% of N_2O are similar to pure CO_2 properties in the whole range of studied temperatures (273 – 293 K), in agreement with available experimental data. Calculations of CO_2+NO equilibrium and transport properties were also performed at three different temperatures in the range 253 – 273 K. At such temperatures, only the monomer form of the nitric oxide (NO) has to be accounted for. The performed calculations are pure predictions since no experimental data are available in the open literature for this system. For a mixture containing 10 mol% of NO, the simulation results show a decrease of the liquid density and viscosity values of 9% and 24% with respect to corresponding pure CO_2 values, respectively.